

chain nodes : 7 9 10 11 12 13 17 18 20 21 24 25 26 ring nodes :

1 2 3 4 5 6

chain bonds : 1-18 2-25 3-26 4-7 5-17 6-24 9-10 11-12 11-13 20-21

ring bonds : 1-2 1-6 2-3 3-4 4-5 5-6

exact/norm bonds :

1-18 2-25 3-26 4-7 5-17 6-24 9-10 11-12 11-13 20-21 normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6

G1:[@1],[@2]

G2:H,X,Ak,[@1],[@2],[@3]

Hydrogen count :

7:>= minimum 1 Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 9:CLASS 10:CLASS 11:CLASS 12:CLASS 13:CLASS 17:CLASS 18:CLASS 20:CLASS 21:CLASS 24:CLASS 25:CLASS 26:CLASS